On Dalgarno and Lewis Perturbation Theory for Scattering States

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Abstract

We apply the method of Dalgarno and Lewis to scattering states and discuss the choice of the unperturbed model in order to have a convergent perturbation series for the phase shift.

1 Introduction

There has been some interest in the application of on–shell perturbation theory to simple scattering problems in one dimension [1–3]. Those approaches were mainly based on logarithmic perturbation theory [1] and the Dalgarno–Lewis perturbation theory [2, 3]. In order to bypass the problem posed by the nodes of real wavefunctions they used complex wavefunctions (Jost functions). Although the method of Dalgarno and Lewis was proposed as a device to calculate sum over states [4] it proves to be an efficient approach for on–shell perturbation theory [5, 6]. This method has recently been applied to

solve the differential equation for the density distribution in scattering problems [7].

The purpose of this paper is to discuss the application of the Dalgarno and Lewis perturbation theory to potential scattering using real wavefunctions. We also consider the choice of the unperturbed or reference model in order to have convergent perturbation series for the phase shift. In Sec. 2 we introduce the model. In Sec. 3 we propose an alternative application of the method of Dalgarno and Steward and a choice of the unperturbed model potential. In Sec. 4 we apply the main equations to an illustrative example, and in Sec. 6 we summarize the main results of the paper and draw some conclusions.

2 The model

For simplicity we consider the one–dimensional model

$$-\frac{\hbar^2}{2m}\psi''(r) + V(r)\psi(r) = E\psi(r) \tag{1}$$

and choose the boundary condition $\psi(0) = 0$ in order to mimic the s–states of a central–field model. The prime denotes differentiation with respect to the coordinate. The potential–energy function $V(r)$ is negative for $r < L$ and zero for $r \geq L$. In order to derive a dimensionless differential equation we define the new independent variable $x = r/L$ and rewrite Eq. (1) as

$$y''(x) = [v(x) - \epsilon]y(x) \tag{2}$$

where

$$v(x) = \frac{2m}{\hbar^2}V(Lx),\ \epsilon = \frac{2m}{\hbar^2}E,\ y(x) = \psi(Lx). \tag{3}$$

The boundary conditions are

$$y(0) = 0,\ y(x) = \frac{1}{k}\sin(kx + \delta),\ x > 1 \tag{4}$$

where δ is the phase shift and $k = \sqrt{\epsilon}$. In order to avoid ambiguities regarding to multiples of π we choose $\delta(k)$ to satisfiy $\delta(\infty) = 0$.

In order to apply perturbation theory we choose a closely related problem

$$y_0''(x) = [v_0(x) - \epsilon]y_0(x) \tag{5}$$

with similar boundary conditions

$$y_0(0) = 0,\ y_0(x) = \frac{1}{k}\sin(kx + \delta_0),\ x > 1. \tag{6}$$

As it is custommary in most applications of perturbation theory we write $v(x) = v_0(x) + \lambda v_1(x)$, where the perturbation parameter λ is set equal to unity at the end of the calculation, and expand

$$\begin{aligned} y(x) &= \sum_{j=0}^{\infty} y_j(x)\lambda^j, \\ \delta &= \sum_{j=0}^{\infty} \delta_j \lambda^j. \end{aligned} \tag{7}$$

3 The method of Dalgarno and Lewis

For simplicity we write $Q(x) = v(x) - \epsilon$, and $Q_0(x) = v_0(x) - \epsilon$. The function $F(x) = y(x)/y_0(x)$ satisfies the differential equation

$$\left(y_0(x)^2 F'(x)\right)' = \Delta Q(x) F(x) y_0(x)^2 \tag{8}$$

where $\Delta Q = Q - Q_0$. Since the nodes of $y(x)$ and $y_0(x)$ do not coincide one expects $F(x)$ to have poles at the nodes of $y_0(x)$. However, $F(x)$ does not appear in the resulting expression for $y(x)$ (see below) and, consequently, that problem does not arise in practical applications of the method of Dalgarno and Lewis.

Notice that

$$y_0(x)^2 F'(x) = y'(x)y_0(x) - y(x)y_0'(x) = W(y, y_0)(x) \tag{9}$$

is the Wronskian of the perturbed and unperturbed solutions. On integrating Eq. (8) we have

$$W(y, y_0)(x) = \int_0^x \left(\Delta Q y y_0\right)(x')\, dx'. \tag{10}$$

At $x = 1$ we substitute the asymptotic forms of $y(x)$ and $y_0(x)$ into the Wronskian and obtain an expression for the phase shift

$$\sin(\Delta\delta) = -k \int_0^1 \left(\Delta Q y y_0\right)(x)\, dx. \tag{11}$$

If we integrate Eq. (10) between $x = 1$ and x and multiply the result by $y_0(x)$ we obtain an expression for $y(x)$:

$$y(x) = Cy_0(x) + y_0(x) \int_1^x \frac{dx'}{y_0(x')^2} \int_0^{x'} (\Delta Q y y_0)(x'')\, dx'' \tag{12}$$

where C is an integration constant. Notice that this expression is free from poles because the function $F(x)$ does not appear explicitly in it.

When $x > 1$ then $x' > 1$ and we substitute Eq. (11) for the second integral in Eq. (12). Moreover, in order to have the correct asymptotic expression for $y(x)$ the integration constant should be

$$C = \sin(\Delta\delta)\cot(k + \delta_0) + \cos(\Delta\delta) \tag{13}$$

that we also expand in a power series: $C = 1 + C_1\lambda + C_2\lambda^2 + \ldots$

Finally, it follows from equations (11), (12), and (13) that

$$y_j(x) = C_j y_0(x) + y_0(x) \int_1^x \frac{dx'}{y_0(x')^2} \int_0^{x'} (v_1 y_{j-1} y_0)(x'')\, dx'' \tag{14}$$

$$\begin{aligned}
\delta_1 &= -k \int_0^1 v_1(x) y_0(x)^2\, dx \\
\delta_2 &= -k \int_0^1 v_1(x) y_0(x) y_1(x)\, dx \\
\delta_3 &= \frac{\delta_1^3}{6} - k \int_0^1 v_1(x) y_0(x) y_2(x)\, dx
\end{aligned} \tag{15}$$

and

$$\begin{aligned}
C_1 &= \delta_1 \cot(k + \delta_0) \\
C_2 &= \delta_2 \cot(k + \delta_0) - \frac{\delta_1^2}{2} \\
C_3 &= \left(\delta_3 - \frac{\delta_1^3}{6}\right) \cot(k + \delta_0) - \delta_1\delta_2.
\end{aligned} \tag{16}$$

At the jth perturbation step we first solve for $y_j(x)$ and δ_j and then calculate C_j. Those expressions are sufficient for present discussion, one can easily derive as many as necessary from the equations above.

The number of necessary perturbation corrections depends on the convergence rate of the perturbation series. For that reason it is important to

choose a convenient unperturbed or reference potential $v_0(x)$. It has been argued that in order to have an adequate rate of convercence the unperturbed and perturbed potentials should support the same number of bound states [1]. This conclusion is based on Levinson's theorem than in our case takes the form $\delta(k=0) = N\pi$, where N is the number of bound states [8]. Here we investigate the application of the Bargmann–Schwinger upper limit to the number of bound states [9, 10] and require that at least

$$\int_0^1 v_0(x)\,dx = \int_0^1 v(x)\,dx. \tag{17}$$

Although this condition does not completely guarantee that both potentials have the same number of bound states, it is a reasonable choice that will prove sound in the example below.

The simplest exactly solvable unperturbed model is one with a constant potential

$$v_0(x) = \begin{cases} -v_0 \; if \; 0 < x < 1 \\ 0 \; if \; x \geq 1 \end{cases} \tag{18}$$

in which case

$$v_0 = -\int_0^1 v(x)\,dx.$$

The starting–point of the calculation are the unperturbed solutions

$$\begin{aligned} y_0(x) &= \frac{\sin(k+\delta_0)}{k\sin(K)}\sin(Kx),\ 0 < x < 1, \\ K &= \sqrt{k^2 + v_0}, \\ \delta_0 &= \arctan\left(\frac{k\tan(K)}{K}\right) - k + n\pi \end{aligned} \tag{19}$$

where we choose n so that $\delta_0(k \to \infty) = 0$ as stated above.

4 Example

In what follows we compare the perturbation results with accurate numerical phase shifts calculated by a straightforward power–series method. To this end we assume that the Taylor series of the potential around $x = 0$, $v(x) = w_0 + w_1 x + \ldots$ converges at $x = 1$, and expand the solution in the same way:

$y(k,x) = c_0(k) + c_1(k)x + c_2(k)x^2 + \ldots$, where $c_0 = c_2 = 0$ and $c_j(k,c_1) = c_j(k,1)c_1$, $j = 3,4,\ldots$. Finally, we obtain the phase shift as

$$\delta = \arctan\left(\frac{y(k,1)}{y'(k,1)}\right) - k + n\pi. \tag{20}$$

As an illustrative example, we choose

$$v(x) = Ax(x-1),\ A > 0,\ 0 < x < 1 \tag{21}$$

that can be solved in terms of confluent hypergeometric functions [11]. However, here we resort to the power series approach because it is suitable for more general problems and converges fast in most cases. The power–series approach also enables us to obtain the bound–state energies from the conditon

$$y'(k,1) + ky(k,1) = 0,\ k = \sqrt{-\epsilon} \tag{22}$$

We choose a well of depth v_0 as unperturbed model and the simple condition (17) gives us $v_0 = A/6$. We could obtain analytical expressions for $\delta_1(A,v_0,\delta_0)$, $\delta_2(A,v_0,\delta_0)$ and $\delta_3(A,v_0,\delta_0)$ but we only show the first perturbation correction because the other ones are too long.

$$\begin{aligned}
\delta_1 \;=\; & \frac{\sin(\delta_0+k)^2}{12k(k^2+v_0)^{3/2}\sin\left(\sqrt{k^2+v_0}\right)^2} \\
& \left\{3\left[a - 2v_0\left(k^2+v_0\right)\right]\sin\left(\sqrt{k^2+v_0}\right)\cos\left(\sqrt{k^2+v_0}\right)\right. \\
& +\sqrt{k^2+v_0}\left[3a\sin\left(\sqrt{k^2+v_0}\right)^2 - a\left(k^2+v_0+3\right)\right. \\
& \left.\left.+6v_0\left(k^2+v_0\right)\right]\right\}
\end{aligned} \tag{23}$$

In order to test the accuracy of perturbation theory we choose parabolic wells with $A = 6$ with no bound states, and $A = 18$ with one bound state. Figures 1 and 2 show the logarithmic error $\epsilon_{\log} = \log|(\delta_{PS} - \delta_{PT})/\delta_{PS}|$, where PS and PT denote power series and perturbation theory, respectively. We clearly appreciate that the perturbation series converges for both parabolic–well strengths, and for all energies. For some k values the perturbation series of order $j-1$ may be more accurate than the one of order j. We do not know if this behaviour is fortuitous or if there is a mathematical or physical reason behind. Table 1 shows the average relative error $\epsilon_{av} = \frac{1}{M}\sum_{j=1}^{M}|[\delta_{PS}(k_j) - \delta_{PT}(k_j)]/\delta_{PS}(k_j)|$ for some A–values. We clearly appreciate that the perturbation series converges smoothly.

5 More general problems

One can easily apply the method of Dalgarno and Steward to more general problems of the form

$$y''(x) = Q(y, x) \tag{24}$$

where $Q(y, x)$ denotes a differential operation on $y(x)$. We choose a convenient unperturbed problem

$$y_0''(x) = Q_0(y_0, x) \tag{25}$$

and proceed as in Sec. 2. We obtain the following general equation

$$\begin{aligned} y(x) &= C_2 y_0(x) + C_1 y_0(x) \int_\beta^x \frac{dx'}{y_0(x')^2} \\ &\quad + y_0(x) \int_\beta^x \frac{dx'}{y_0(x')^2} \int_\alpha^x \left(Q y_0 - Q_0 y\right)(x'')\, dx'' \end{aligned} \tag{26}$$

where we can choose the arbitrary integration limits α and β and constants C_1, and C_2, conveniently according to the problem.

Notice that if $Q_0(y_0, x) = Q_0(x) y_0(x)$ then

$$u(x) = y_0(x) \int_\beta^x \frac{dx'}{y_0(x')^2} \tag{27}$$

is a solution of $u''(x) = Q_0(x) u(x)$ and $W(u, y_0) = 1$. That is to say, $y_0(x)$ and $u(x)$ are two independent solutions of the unperturbed model.

It is not difficult to verify that the method of Dalgarno and Lewis applies to velocity–dependent problems [13]. If we choose

$$\begin{aligned} Q(y, x) &= [v_0(x) + \lambda v_1(x) - \epsilon] y(x) + \lambda \rho(x) y''(x) \\ &\quad - \lambda \left[y'(x) - \frac{y(x)}{x} \right] \rho'(x) \end{aligned} \tag{28}$$

then we have the model treated by Jaghoub [13]. Therefore, if

$$Q_0(y_0, x) = [v_0(x) - \epsilon_0] y_0(x) \tag{29}$$

we have

$$\begin{aligned} Q y_0 - Q_0 y &= -\Delta\epsilon y y_0 + \lambda v_1 y y_0 + \lambda \rho y_0 y'' \\ &\quad - \lambda \left[y' - \frac{y}{x} \right] \rho' y_0. \end{aligned} \tag{30}$$

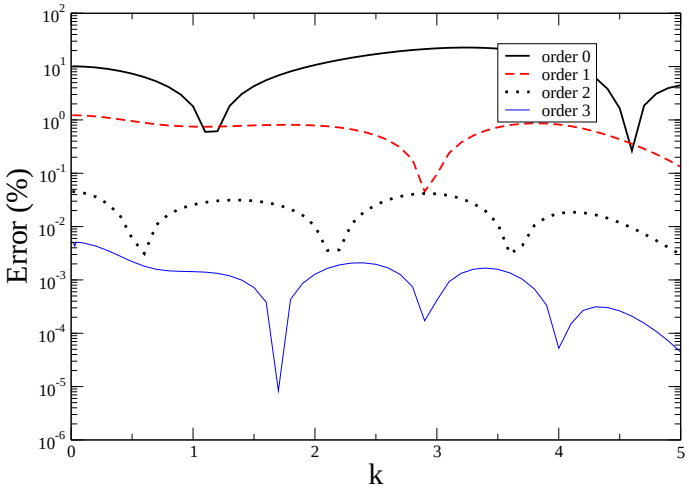

Figure 1: The error $\epsilon = \left|\frac{\delta_{PS}-\delta_{PT}}{\delta_{PS}}\right| \times 100$ for $A = 6$.

If we expand $y(x)$ as in Eq. (7) and $\Delta\epsilon = \epsilon_1\lambda + \epsilon_2\lambda^2 + \ldots$ then we obtain Jaghoub's perturbation equations [13] provided that we choose the arbitrary constants conveniently. In other words: Jaghoub's procedure is merely the method of Dalgarno and Lewis for bound states developed in a different way.

By means of the equations displayed above, the reader can easily verify that present implementation of the method of Dalgarno and Lewis is also suitable for the treatment of scattering problems with velocity–dependent interactions [12].

6 Conclusions

We have shown that the method of Dalgarno and Lewis is suitable for the calculation of phase shifts by means of perturbation theory. One can use real eigenfunctions because their nodes do not cause the occurrence of poles into the solutions.

The constant potential is a suitable unperturbed or reference model for the application of perturbation theory to some problems. A simple prescription for the well–depth leads to reasonable convergence rate and enables one to obtain accurate results with perturbation series of low order.

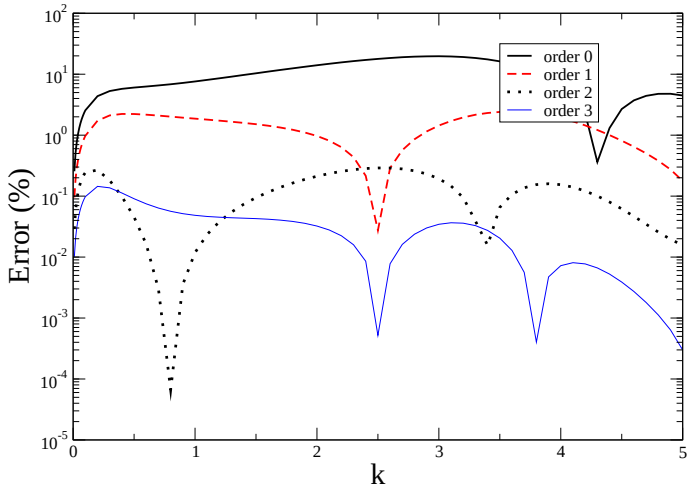

Figure 2: The error $\epsilon = \left|\frac{\delta_{PS}-\delta_{PT}}{\delta_{PS}}\right| \times 100$ for $A = 18$.

Table 1: Average relative error for the parabolic well $V(x) = Ax(x-1)$

A	Zeroth order	First order	Second order	Third order
6	0.1060	0.00736	0.00024	0.000018
12	0.0917	0.02250	0.00106	0.000672
18	0.0906	0.01260	0.00127	0.000365
24	0.0814	0.01109	0.00200	0.000327

We have shown that the method of Dalgarno and Lewis also applies to bound–state and scattering problems with velocity–dependent interactions [12, 13].

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